A Simplified Crossover SAFT Equation of State for Hydrofluorocarbon Mixtures

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It is well known that all analytical equations of state fail to reproduce the non-analytical, singular behavior of fluids in the critical region, caused by long-scale fluctuations in density. A generalized crossover approach for the incorporation of the effects of the critical fluctuations into a classical – analytical equation of state has been developed recently [1]. This approach based on the fundamental results of the renormalization-group theory and has been previously successfully applied to the cubic Patel-Teja (PT) EOS [2] and to the statistical associating fluid theory (SAFT) EOS [3]. In this work a simplified modification of the crossover SAFT EOS is used to describe thermodynamic properties of pure refrigerants and binary refrigerant mixtures in the wide range of parameters of state including the nearest vicinity of the critical point. For pure components, the simplified crossover (SCR) SAFT model contains only three system-dependent parameters but allows an accurate prediction of the critical parameters of pure fluids and yields a better representation of the thermodynamic properties of pure fluids than the original SAFT equation of state. For binary mixtures, the simple mixing rules with only one adjustable parameter are used.

A comparison is made with experimental data for pure refrigerants R12, R22, R32, R125, R134a, R143a, and mixtures R22+R12, R32+R134a and R125+R32 in the one- and two-phase regions. The SCR SAFT EOS reproduces the saturated pressure data with an average absolute deviation (AAD) of about 1.1% and the saturated liquid densities with an AAD of about 0.9%. In the one-phase region, the SCR SAFT equation represents the experimental values of pressure with AAD of about 2.2% in the range of temperatures and density bounded by $T \ge T_c$ and $\rho \le 2\rho_c$.

- [1] S.B. Kiselev, Fluid Phase Equilib. **147**, 7 (1998).
- [2] N.C. Patel and A.S. Teja, Chem. Eng. Sci. 27, 463 (1982).
- [3] H.S. Huang and M. Radosz, Ind. Eng. Chem. Res. 98, 10634 (1994).